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The quantal Poincaré–Cartan integral invariant for singular higher-order Lagrangian in field theories

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Abstract. Based on the phase-space generating functional of the Green function for a system with a regular/singular higher-order Lagrangian, the quantal Poincaré–Cartan integral invariant (QPCII) for the higher-order Lagrangian in field theories is derived. It is shown that this QPCII is equivalent to the quantal canonical equations. For the case in which the Jacobian of the transformation may not be equal to unity, the QPCII can still be derived. This case is different from the quantal first Noether theorem. The relations between QPCII and a canonical transformation and those between QPCII and the Hamilton–Jacobi equation at the quantum level are also discussed.

1 Introduction

A dynamical system described by a higher-order Lagrangian was first given by Ostrogradsky. Recently, it has attracted much attention because higher-order derivative theories have close relations with modern field theories, relativistic particle dynamics, gravity theory, modified Korteweg–de Vries (KDV) equations, supersymmetry, the string model and other problems.

In quantum theories, the path-integral quantization can be used as well as the formulation of canonical (operator) quantization. The two formulations are equivalent. In the formulation of path-integral quantization, the main ingredient is the classical action together with the measure in the space of field configurations. Thus, path integrals provide a useful tool in the study of the symmetries at the quantum level. The phase-space path integrals are more fundamental than the configuration-space path integrals [1].

The classical Poincaré–Cartan integral invariant (CPCII) plays a fundamental role in classical mechanics and field theories. Based on CPCII, it follows that the classical equations of motion of the dynamical system are Hamilton canonical equations. CPCII can be treated as a fundamental principle of a dynamical system in classical theories [2,3]. For a regular/singular system, the CPCII is equivalent to the classical canonical equations. CPCII has been generalized to non-holonomic systems at the classical level [4,5]. In addition, the CPCII for a system with a singular Lagrangian has been studied by some authors and some applications are also given [6–9]. However, these investigations of the CPCII for the system are developed at the classical level [10,11]. It needs further study whether they hold true at the quantum level or not. The preliminary discussion of QPCII for the system with finite degrees of freedom has been given in [12]. However, the symbol of the ground state still appears in those QPCII. In this paper we shall study QPCII for the system with high-order Lagrangian in field theories, and the symbol of the ground state will disappear.

This paper is organized as follows. In the beginning of Sect. 2, we start this section by reviewing very briefly the Ostrogradsky transformation for a higher-order Lagrangian. Then the QPCII for the higher-order derivative Lagrangian in field theories is derived in which the Jacobian of the transformation may not be equal to unity. The symbol of the vacuum state of the field is eliminated. This case is different from the quantal first Noether theorem [7]. In Sect. 3, the equivalence between QPCII and quantal canonical equations is pointed out. In Sect. 4, the connection between the canonical transformation at the quantum level and the QPCII is given. In Sect. 5, the Hamilton–Jacobi equation at the quantum level derived from QPCII is discussed. Section 6 is devoted to the conclusion, the comparisons of the results at the quantum level and those in classical theories are discussed.

2 The quantal Poincaré–Cartan integral invariant

Let us first consider a system with a regular higher-order Lagrangian described by the field variables $\psi^\alpha(x)(\alpha = 1, 2, \ldots, n)$, $x = (x_0, x_i)(x_0 = t, i = 1, 2, 3)$. The motion of the field is described by a regular Lagrangian involv-

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ing higher-order derivatives of the field variables, and the Lagrangian of the system is given by

$$L[\psi^\alpha_{(0)}, \psi^\alpha_{(1)}, \dots \psi^\alpha_{(N)}] = \int \mathcal{L}(\psi^\alpha, \psi^\alpha_{,\mu}, \dots \psi^\alpha_{,\mu(N)})\mathrm{d}^3x, \quad (1)$$

where $\psi^\alpha_{(0)} = \psi^\alpha, \psi^\alpha_{(1)} = \dot{\psi}^\alpha, \dots, \psi^\alpha_{,\mu} = \partial_\mu\psi^\alpha, \psi^\alpha_{,\mu(m)} = \underbrace{\partial_\mu\partial_\nu\dots\partial_\rho}_{m}\psi^\alpha$, and V is the space domain of the field. The flat space-time metric is $g_{\mu\nu} = (1, -1, -1, -1)$. Using the Ostrogradsky transformation, one can introduce generalized canonical momenta:

$$\pi_\alpha^{(N-1)} = \frac{\delta L}{\delta\psi^\alpha_{(N)}}, \quad (2a)$$

$$\pi_\alpha^{(s-1)} = \frac{\delta L}{\delta\psi^\alpha_{(s)}} - \dot{\pi}_\alpha^{(s)} \quad (s = 1, 2, \dots, N-1), \quad (2b)$$

or

$$\pi_\alpha^{(s-1)} = \sum_{j=0}^{N-s} (-1)^j \frac{\mathrm{d}^j}{\mathrm{d}t^j} \frac{\delta L}{\delta\psi^\alpha_{(j+s)}} \quad (s = 1, 2, \dots, N-1), \quad (3)$$

and using these relations one can go over from the Lagrangian description to the Hamiltonian description. The generalized canonical Hamiltonian is defined by

$$H_\mathrm{c}[\psi^\alpha_{(s)}, \pi_\alpha^{(s)}] = \int \mathcal{H}_\mathrm{c}\mathrm{d}^3x = \int (\pi_\alpha^{(s)}\psi^\alpha_{(s+1)} - \mathcal{L})\mathrm{d}^3x \quad (4)$$

which may be formed by eliminating only the highest derivatives $\psi^\alpha_{(N)}$. A summation over the indices α from 1 to n and s from 0 to $N-1$ is taken repeatedly.

The generating functional of the Green function in phase space for this system can be written as [7]

$$Z[J, K] = \int \mathcal{D}\psi^\alpha_{(s)}\mathcal{D}\pi^\alpha_{(s)} \times \exp\left\{\mathrm{i}\left[I^P + \int \mathrm{d}^4x(J^s_\alpha\psi^\alpha_{(s)} + K^\alpha_s\pi_\alpha^{(s)})\right]\right\}, \quad (5)$$

where $I^p = \int \mathrm{d}^4x\mathcal{L}^p = \int \mathrm{d}^4x(\pi_\alpha^{(s)}\psi^\alpha_{(s+1)} - \mathcal{H}_\mathrm{c})$. $J_\alpha(x)$ and $K^\alpha(x)$ are exterior sources with respect to the fields $\psi^\alpha(x)$ and their canonical momenta $\pi_\alpha(x)$, respectively.

We consider the space coordinates x_i to be a fixed parameter [13]. A "curve" in the phase space is defined by

$$\psi^\alpha_{(s)} = \psi^\alpha_{(s)}(t, \theta), \quad \pi_\alpha^{(s)} = \pi_\alpha^{(s)}(t, \theta), \quad (6)$$

where θ is a parameter. Let us consider the infinitesimal transformation in extended phase space which arises from the change of the parameter θ (x_i is fixed):

$$\begin{cases} t \to t' = t + \Delta t(\theta), \\ \psi^\alpha_{(s)}(t, x_i) \to {\psi'}^\alpha_{(s)}(t', x_i) \\ \qquad = \psi^\alpha_{(s)}(t, x_i) + \Delta\psi^\alpha_{(s)}(t, x_i, \theta), \\ \pi_\alpha^{(s)}(t, x_i) \to {\pi'}_\alpha^{(s)}(t', x_i) \\ \qquad = \pi_\alpha^{(s)}(t, x_i) + \Delta\pi_\alpha^{(s)}(t, x_i, \theta), \end{cases} \quad (7)$$

where θ satisfies

$${\psi'}^\alpha_{(s)}(t, x_i, 0) = \psi^\alpha(t, x_i), \quad {\pi'}_\alpha^{(s)}(t, x_i, 0) = \pi_\alpha(t, x_i). \quad (8)$$

Under the transformation (7), the variation of the canonical action is given by

$$\Delta I^p = \int \mathrm{d}^4x \left(\frac{\delta I^P}{\delta\psi^\alpha_{(s)}}\delta\psi^\alpha_{(s)} + \frac{\delta I^p}{\delta\pi_\alpha^{(s)}}\delta\pi_\alpha^{(s)}\right) + \int \mathrm{d}^4x \left\{\partial_\mu[(\pi_\alpha^{(s)}\psi^\alpha_{(s+1)} - \mathcal{H}_\mathrm{c})\Delta x^\mu] + \frac{\mathrm{d}}{\mathrm{d}t}(\pi_\alpha^{(s)}\delta\psi^\alpha_{(s)})\right\}, \quad (9)$$

where

$$\frac{\delta I^p}{\delta\psi^\alpha_{(s)}} = -\dot{\pi}_\alpha^{(s)} - \frac{\delta H_\mathrm{c}}{\delta\psi^\alpha_{(s)}}, \quad \frac{\delta I^p}{\delta\pi_\alpha^{(s)}} = \dot{\psi}^\alpha_{(s)} - \frac{\delta H_\mathrm{c}}{\delta\pi_\alpha^{(s)}}, \quad (10)$$

and H_c is a generalized canonical Hamiltonian. The relations between the substantial variations $\delta\psi^\alpha_{(s)}$, $\delta\pi_\alpha^{(s)}$ and the total variations $\Delta\psi^\alpha_{(s)}$, $\Delta\pi_\alpha^{(s)}$ are given by

$$\delta\psi^\alpha_{(s)} = \Delta\psi^\alpha_{(s)} - \psi^\alpha_{(s),\mu}\Delta x^\mu = \Delta\psi^\alpha_{(s)} - \psi^\alpha_{(s),0}\Delta x^0, \quad (11a)$$

$$\delta\pi_\alpha^{(s)} = \Delta\pi_\alpha^{(s)} - \pi^{(s)}_{\alpha,\mu}\Delta x^\mu = \Delta\pi_\alpha^{(s)} - \pi^{(s)}_{\alpha,0}\Delta x^0. \quad (11b)$$

Let it be supposed that the Jacobian of the transformation (7) of the field variables is given by $\bar{J}(\theta) = 1 + J_1(\theta)(\bar{J}(0) = 1)$. The smoothed function $J_1(\theta)$ can be expressed by using a total differential function $Q(\theta)$ i.e. $J_1(\theta) = \mathrm{d}Q(\theta)/\mathrm{d}\theta$. The generating function of the Green function is invariant under the transformation (7) which can be written as

$$\begin{aligned} Z[J, K] = \int &\mathcal{D}\psi^\alpha_{(s)}\mathcal{D}\pi_\alpha^{(s)} \\ &\times \left\{1 + J_1 + \mathrm{i}\int \mathrm{d}x^4 \left[\left(\frac{\delta I^P}{\delta\psi^\alpha_{(s)}} + J^s_\alpha\right)\delta\psi^\alpha_{(s)} + \left(\frac{\delta I^p}{\delta\pi_\alpha^{(s)}} + K^\alpha_s\right)\delta\pi_\alpha^{(s)}\right]\right. \\ &\left. + \mathrm{i}\int \mathrm{d}x^4\{\partial_\mu[(\pi_\alpha^{(s)}\psi^\alpha_{(s+1)} - \mathcal{H}_\mathrm{c})\Delta x^\mu] + \frac{\mathrm{d}}{\mathrm{d}t}(\pi_\alpha^{(s)}\delta\psi^\alpha_{(s)})\right\} \\ &\times \exp\left\{\mathrm{i}\left[I^p + \int \mathrm{d}x^4(J^s_\alpha\psi^\alpha_{(s)} + K^\alpha_s\pi_\alpha^{(s)})\right]\right\}. \quad (12) \end{aligned}$$

From the invariance of the generating functional (5) under the transformation (7), one obtains

$$\int \mathcal{D}\psi^\alpha_{(s)}\mathcal{D}\pi_\alpha^{(s)} \left\{J_1 + \mathrm{i}\int \mathrm{d}x^4 \left[\left(\frac{\delta I^P}{\delta\psi^\alpha_{(s)}} + J^s_\alpha\right)\delta\psi^\alpha_{(s)} + \left(\frac{\delta I^p}{\delta\pi_\alpha} + K^\alpha_s\right)\delta\pi_\alpha^{(s)}\right] + \mathrm{i}\int \mathrm{d}x^4\{\partial_\mu[(\pi_\alpha^{(s)}\psi^\alpha_{(s+1)} - \mathcal{H}_\mathrm{c})\Delta x^\mu] + \frac{\mathrm{d}}{\mathrm{d}t}(\pi_\alpha^{(s)}\delta\psi^\alpha_{(s)})\}\right\}$$

$$\times \exp\left\{\mathrm{i}\left[I^p + \int \mathrm{d}x^4 (J^s_\alpha \psi^\alpha_{(s)} + K^\alpha_s \pi^{(s)}_\alpha)\right]\right\} = 0. \quad (13)$$

Functionally differentiating (13) with respect to J^s_α, one obtains

$$\int \mathcal{D}\psi^\alpha_{(s)} \mathcal{D}\pi^{(s)}_\alpha \left(\left\{\mathrm{i}J_1 - \int \mathrm{d}x^4 \left[\left(\frac{\delta I^P}{\delta \psi^\alpha_{(s)}} + J^s_\alpha\right)\delta\psi^\alpha_{(s)} + \left(\frac{\delta I^p}{\delta \pi^{(s)}_\alpha} + K^\alpha_s\right)\delta\pi^{(s)}_\alpha\right] - \int \mathrm{d}x^4 \{\partial_\mu[(\pi^{(s)}_\alpha \psi^\alpha_{(s+1)} - \mathcal{H}_\mathrm{c})\Delta x^\mu] + \frac{\mathrm{d}}{\mathrm{d}t}(\pi^{(s)}_\alpha \delta\psi^\alpha_{(s)})\}\right\} \times \psi^\alpha_{(s)}(x_1) + \mathrm{i}\int \mathrm{d}x^4\, \delta(x - x_1) N^{\alpha\sigma}_s\right) \times \exp\left\{\mathrm{i}\left[I^p + \int \mathrm{d}x^4 (J^s_\alpha \psi^\alpha_{(s)} + K^\alpha_s \pi^{(s)}_\alpha)\right]\right\} = 0, \quad (14)$$

where

$$N^{\alpha\sigma}_s = \delta\psi^\alpha_{(s)} = \Delta\psi^\alpha_{(s)} - \psi^\alpha_{(s),0}\Delta x^0. \quad (15)$$

Then, functionally differentiating (13) with respect to J^s_α a total of n times, one gets

$$\int \mathcal{D}\psi^\alpha_{(s)} \mathcal{D}\pi^{(s)}_\alpha \left(\left\{\mathrm{i}\mathrm{d}Q/\mathrm{d}\theta - \int \mathrm{d}x^4 \left[\left(\frac{\delta I^P}{\delta \psi^\alpha_{(s)}} + J^s_\alpha\right)\delta\psi^\alpha_{(s)} + \left(\frac{\delta I^p}{\delta \pi^{(s)}_\alpha} + K^\alpha_s\right)\delta\pi^{(s)}_\alpha\right] - \int \mathrm{d}x^4 \left\{\partial_\mu[(\pi^{(s)}_\alpha \psi^\alpha_{(s+1)} - \mathcal{H}_\mathrm{c})\Delta x^\mu] + \frac{\mathrm{d}}{\mathrm{d}t}(\pi^{(s)}_\alpha \delta\psi^\alpha_{(s+1)})\right\}\right\} \times \psi^\alpha_{(s)}(x_1)\psi^\alpha_{(s)}(x_2)\dots\psi^\alpha_{(s)}(x_n) + \mathrm{i}\sum_j \psi^\alpha_{(s)}(x_1)\dots\psi^\alpha_{(s)}(x_{j-1})\psi^\alpha_{(s)}(x_{j+1})\dots \psi^\alpha_{(s)}(x_n) N^{\alpha\sigma}_s + \mathrm{i}N^{\alpha\sigma}_s\right) \quad (16)$$

$$\times \exp\left\{\mathrm{i}\left[I^p + \int \mathrm{d}x^4 (J^{(s)}_\alpha \psi^\alpha_{(s)} + K^\alpha_{(s)} \pi^{(s)}_\alpha)\right]\right\} = 0.$$

Let $J^s_\alpha = K^\alpha_s = 0$ in (16); then one gets [14]

$$\langle 0|\, T^* \left[-\mathrm{i}\mathrm{d}Q/\mathrm{d}\theta + \int \mathrm{d}^4x \left(\frac{\delta I^p}{\delta\psi^\alpha_{(s)}}\delta\psi^\alpha_{(s)} + \frac{\delta I^p}{\delta\pi^{(s)}_\alpha}\delta\pi^{(s)}_\alpha\right)\right] + \int_{t_1}^{t_2} D \int_V \mathrm{d}^3x (\pi^{(s)}_\alpha \Delta\psi^\alpha_{(s)} - \mathcal{H}_\mathrm{c}\Delta t)]\psi^\alpha_{(s)}(x_1)\psi^\alpha_{(s)}(x_2) \dots \psi^\alpha_{(s)}(x_n)\,|0\rangle - \mathrm{i}\,\langle 0| \left[\sum_j \psi^\alpha_{(s)}(x_1)\dots\psi^\alpha_{(s)}(x_{j-1})\psi^\alpha_{(s)}(x_{j+1}) \dots\psi^\alpha_{(s)}(x_n)N^{\alpha\sigma}_s + N^{\alpha\sigma}_s\right] |0\rangle = 0, \quad (17)$$

where the symbol T^* stands for the covariantized T product [14], $|0\rangle$ is the vacuum state of the field, $D = \frac{\mathrm{d}}{\mathrm{d}t}$. From (15), one can see that the smoothed function of θ can also be expressed as

$$\langle 0| \sum_j \psi^\alpha_{(s)}(x_1)\dots\psi^\alpha_{(s)}(x_{j-1})\psi^\alpha_{(s)}(x_{j+1}) \dots\psi^\alpha_{(s)}(x_n) \times N^{\alpha\sigma}_s\,|0\rangle = \mathrm{d}F(\theta)/\mathrm{d}\theta, \quad (18a)$$

$$\langle 0|\, N^{\alpha\sigma}_s\,|0\rangle = \mathrm{d}G(\theta)/\mathrm{d}\theta. \quad (18b)$$

Fixing t and letting $t_1, t_2, \dots, t_m \to +\infty$, $t_{m+1}, t_{m+2}, \dots, t_n \to -\infty$, noting that $\psi^\alpha_{(s)}(\vec{x}, -\infty)\,|0\rangle = |1, \mathrm{in}\rangle$, $\langle 0|\,\psi^\alpha_{(s)}(\vec{x}, \infty) = \langle \mathrm{out}, 1|$ and using the reduction formula [14], one can write the expression (17) as

$$\langle \mathrm{out}, m|\, T^* \left[\int \mathrm{d}^4x \left(\frac{\delta I^p}{\delta\psi^\alpha_{(s)}}\delta\psi^\alpha_{(s)} + \frac{\delta I^p}{\delta\pi^{(s)}_\alpha}\delta\pi^{(s)}_\alpha\right)\right] |\mathrm{out}, m\rangle + \langle \mathrm{out}, m| \left[\int_V \mathrm{d}^3x \left(\pi^{(s)}_\alpha \Delta\psi^\alpha_{(s)} - \mathcal{H}_\mathrm{c}\Delta t\right)\right] |n - m, \mathrm{in}\rangle|_{t_1} - \langle \mathrm{out}, m| \left[\int_V \mathrm{d}^3x \left(\pi^{(s)}_\alpha \Delta\psi^\alpha_{(s)} - \mathcal{H}_\mathrm{c}\Delta t\right)\right] |n - m, \mathrm{in}\rangle|_{t_2} = \mathrm{i}\{\mathrm{d}F/\mathrm{d}\theta + \mathrm{d}G/\mathrm{d}\theta + \langle \mathrm{out}, m|\, \mathrm{d}Q/\mathrm{d}\theta\,|n - m, \mathrm{in}\rangle\}. \quad (19)$$

Let C_1 be any simple closed curve encircling the tube of quantal dynamical trajectories in extended phase space. $\theta = 0$ and $\theta = l$ are same points on C_1. Through any point on C_1, there is a dynamical trajectory of the motion. The dynamical trajectories through points on C_1 form a tube of trajectories. Choose another closed curve C_2 on this tube of trajectories such that it encircles this tube and intersects the generatrix of the tube only once. Taking the integral of the expression (19) with respect to θ along curves C_1 and C_2[2], one has

$$\oint_{c_1} \langle \mathrm{out}, m|\, T^* \left[\int_V \mathrm{d}^3x \left(\pi^{(s)}_\alpha \Delta\psi^\alpha_{(s)} - \mathcal{H}_\mathrm{c}\Delta t\right)\right] |n - m, \mathrm{in}\rangle\,|_{t_1} - \oint_{c_2} \langle \mathrm{out}, m|\, T^* \left[\int_V \mathrm{d}^3x \left(\pi^{(s)}_\alpha \Delta\psi^\alpha_{(s)} - \mathcal{H}_\mathrm{c}\Delta t\right)\right] |n - m, \mathrm{in}\rangle\,|_{t_2} + \oint_c \langle \mathrm{out}, m|\, T^* \left[\int \mathrm{d}^4x \left(\frac{\delta I^p}{\delta\psi^\alpha_{(s)}}\delta\psi^\alpha_{(s)} + \frac{\delta I^p}{\delta\pi^{(s)}_\alpha}\delta\pi^{(s)}_\alpha\right)\right] |n - m, \mathrm{in}\rangle \quad (20)$$

$$= \mathrm{i}\oint_{c_k} \{[\mathrm{d}F/\mathrm{d}\theta + \mathrm{d}G/\mathrm{d}\theta] + \langle \mathrm{out}, m|\, \mathrm{d}Q/\mathrm{d}\theta\,|n - m, \mathrm{in}\rangle\}.$$

Since $\theta = 0$ and $\theta = l$ are same points on the closed curve, along those closed curves, the integral of the right-hand side of (20) must be equal to zero. Due to m and n being arbitrary, we have

$$\oint_{c_1} T^* \left[\int_V \mathrm{d}^3x \left(\pi^{(s)}_\alpha \Delta\psi^\alpha_{(s)} - \mathcal{H}_\mathrm{c}\Delta t\right)\right] - \oint_{c_2} T^* \left[\int_V \mathrm{d}^3x \left(\pi^{(s)}_\alpha \Delta\psi^\alpha_{(s)} - \mathcal{H}_\mathrm{c}\Delta t\right)\right] + \oint_c T^* \left[\int \mathrm{d}^4x \left(\frac{\delta I^p}{\delta\psi^\alpha_{(s)}}\delta\psi^\alpha_{(s)} + \frac{\delta I^p}{\delta\pi^{(s)}_\alpha}\delta\pi^{(s)}_\alpha\right)\right] = 0. \quad (21)$$

Now, we deduce the quantum canonical equations for this system, since

$$\left\langle \psi'^{\alpha}_{(s)}, t' \right| \frac{\delta I^p}{\delta \psi^{\alpha}_{(s)}} \left| \psi^{\alpha}_{(s)}, t \right\rangle = \int \mathcal{D}\psi^{\alpha}_{(s)} \mathcal{D}\pi^{(s)}_{\alpha} \frac{\delta I^p}{\delta \psi^{\alpha}_{(s)}} \exp\{\mathrm{i} I^P\}, \tag{22a}$$

$$\left\langle \psi'^{\alpha}_{(s)}, t' \right| \frac{\delta I^p}{\delta \pi^{(s)}_{\alpha}} \left| \psi^{\alpha}_{(s)}, t \right\rangle = \int \mathcal{D}\psi^{\alpha}_{(s)} \mathcal{D}\pi^{(s)}_{\alpha} \frac{\delta I^p}{\delta \pi^{(s)}_{\alpha}} \exp\{\mathrm{i} I^P\} \tag{22b}$$

for the arbitrary state $\left|\psi'^{\alpha}_{(s)}, t'\right\rangle$ and $\left|\psi^{\alpha}_{(s)}, t\right\rangle$, from the classical canonical equations ($\frac{\delta I^p}{\delta \psi^{\alpha}_{(s)}} = 0$, $\frac{\delta I^p}{\delta \pi^{(s)}_{\alpha}} = 0$), the right-hand side of (22) is equal to zero; thus one can obtain

$$\left\langle \psi'^{\alpha}, t' \right| \frac{\delta I^p}{\delta \psi^{\alpha}_{(s)}} \left| \psi^{\alpha}, t \right\rangle = \left\langle \psi'^{\alpha}, t' \right| \frac{\delta I^p}{\delta \pi^{(s)}_{\alpha}} \left| \psi^{\alpha}, t \right\rangle = 0. \tag{23}$$

Due to $\left|\psi'^{\alpha}, t'\right\rangle$ and $\left|\psi^{\alpha}, t\right\rangle$ being arbitrary, the quantum dynamical trajectories are determined by the following quantal canonical equations:

$$\frac{\delta I^p}{\delta \psi^{\alpha}_{(s)}} = 0, \quad \frac{\delta I^p}{\delta \pi^{(s)}_{\alpha}} = 0. \tag{24}$$

Using the quantal canonical equations (24), from (21), one has

$$W = T^* \oint_c \int_V \mathrm{d}^3 x (\pi^{(s)}_{\alpha} \Delta \psi^{\alpha}_{(s)} - \mathcal{H}_{\mathrm{c}} \Delta t) = \mathrm{inv}. \tag{25}$$

Therefore, with an arbitrary displacement and the deformation of the closed curve C along any tube of those dynamical trajectories, the integral W along the closed curve C is invariant. Equation (25) is called the QPCII for a regular higher-order Lagrangian in field theories and the expression W is a Poincaré–Cartan (PC) integral.

For a system with a singular higher-order Lagrangian, let $\Lambda_k(t, \psi^{\alpha}_{(s)}, \pi^{(s)}_{\alpha}) \approx 0 (k = 1, 2, \ldots, a)$ be first-class constraints, and let $\theta_i(t, \psi^{\alpha}_{(s)}, \pi^{(s)}_{\alpha}) \approx 0 (i = 1, 2, \ldots, b)$ be second-class constraints. The gauge conditions connecting with the first-class constraints are

$$\Omega_l(t, \psi^{\alpha}_{(s)}, \pi^{(s)}_{\alpha}) \approx 0 \quad (l = 1, 2, \ldots, a) .$$

According to the Faddeeve–Senjanovic path-integral quantization scheme, the phase-space generating function of the Green function for the singular higher-order Lagrangian is given by [7]

$$\begin{aligned} Z[J, K] = \int \mathcal{D}\psi^{\alpha}_{(s)} \mathcal{D}\pi^{(s)}_{\alpha} \prod_{i,k,l} \delta(\theta_i) \delta(\Lambda_k) \delta(\Omega_l) \\ \times \det |\{\Lambda_k, \Omega_l\}| \, [\det |\{\theta_i, \theta_j\}|]^{1/2} \\ \times \exp\left\{ \mathrm{i} \left[I^P + \int \mathrm{d}^4 x (J^s_{\alpha} \psi^{\alpha}_{(s)} + K^{\alpha}_s \pi^{(s)}_{\alpha}) \right] \right\}. \end{aligned} \tag{26}$$

Using the properties of the δ-function and the integral properties of the Grassmann variables $C_a(x)$ and $\bar{C}_a(x)$, the expression (26) can be written as

$$\begin{aligned} Z[J, K, \eta^m, \bar{j}, \bar{k}, j, k] \\ = \int \mathcal{D}\psi^{\alpha}_{(s)} \mathcal{D}\pi^{(s)}_{\alpha} \mathcal{D}\lambda_m \mathcal{D}\bar{C}_a \mathcal{D}\pi^a \mathcal{D}C_a \mathcal{D}\bar{\pi}^a \\ \times \exp\left\{ \mathrm{i} \int \mathrm{d}^4 x (\mathcal{L}^P_{\mathrm{eff}} + J^s_{\alpha} \psi^{\alpha}_{(s)} \right. \\ \left. + K^{\alpha}_s \pi^{(s)}_{\alpha} + \eta^m \lambda_m + \bar{j}^a C_a + \bar{C}_a j^a + \bar{k}_a \pi^a + \bar{\pi}^a k_a) \right\}, \end{aligned} \tag{27}$$

where

$$\mathcal{L}^P_{\mathrm{eff}} = \mathcal{L}^P + \mathcal{L}_m + \mathcal{L}_{gh}, \tag{28}$$

$$\mathcal{L}^p = \pi^{(s)}_{\alpha} \psi^{\alpha}_{(s+1)} - \mathcal{H}_{\mathrm{c}}, \tag{29}$$

$$\mathcal{L}_m = \lambda_i \theta_i + \lambda_k \Lambda_k + \lambda_l \Omega_l, \tag{30}$$

$$\begin{aligned} L_{gh} = \int \mathrm{d}^3 y \, [\bar{C}_k(x) \{\Lambda_k(x), \Omega_l(y)\} C_l(y) \\ + \frac{1}{2} \bar{C}^{(}_i x) \{\theta_i(x), \theta_j(y)\} C_j(y) \Big], \end{aligned} \tag{31}$$

and $\lambda_m = (\lambda_k, \lambda_i, \lambda_l)$, λ_k and λ_i and λ_l are multiplier fields connected with the constraints Λ_k,θ_i and Ω_l,respectively. $\bar{\pi}^a(x)$ and $\pi^a(x)$ are canonical momenta conjugate to $C_a(x)$ and $\bar{C}_a(x)$, respectively; here we have introduced the exterior sources η^m,$\bar{j}^a$, $\bar{k}_a$, j^a and k_a with respect to the fields λ_m, C_a, π^a, $\bar{C}_a$ and $\bar{\pi}^a$, respectively. Thus, it is easy to see that the quantal canonical equations are determined by $\mathcal{H}_{\mathrm{eff}} = \pi^{(s)}_{\alpha} \dot{\psi}^{\alpha}_{(s)} - \mathcal{L}^p_{\mathrm{eff}}$ for the system with a singular Lagrangian. Hence, we can still proceed in the same way to obtain the QPCII for the system with a singular higher-order Lagrangian in which the Jacobian of the transformation (7) may not be equal to unity. But in the result for this case, one must use $\mathcal{H}_{\mathrm{eff}}$ instead of $\mathcal{H}_{\mathrm{c}}$ in expression (25):

$$W' = T^* \oint_c \int_V \mathrm{d}^3 x (\pi^{(s)}_{\alpha} \Delta \psi^{\alpha}_{(s)} - \mathcal{H}_{\mathrm{eff}} \Delta t) = \mathrm{inv}. \tag{32}$$

The closed curves must satisfy all the constraint conditions. Thus, we obtain that the QPCII for the singular higher-order Lagrangian can also be derived when we use the effective action I^p_{eff} instead of I^p.

3 Quantal PC integral invariant and quantal canonical equations

In classical theories, it has been proved that CPCII is equivalent to the classical motion equations [7, 10, 11]. In this section, we can show that this equivalent relation at the quantum level still holds true. Now we study the inversion problem of Sect. 2, i.e. the quantal motion equations can be derived from the QPCII for the system with regular/singular higher-order Lagrangian.

Now, we first consider the discrete regular system. We can divide the space domain V into a very large number of small cells and use ΔV_i to denote the volume of the ith cell; $\psi^{\alpha}_{(s)i}$, the average of the variables $\psi^{\alpha}_{(s)}(x)$ on ΔV_i, and $p^{(s)i}_{\alpha}(t)$, the canonical momenta conjugate to $\psi^{\alpha}_{(s)i}$. Thus, $p^{(s)i}_{\alpha}(t) = \pi^{(s)i}_{\alpha} \Delta V_i$ (not summing over i). In this way the discrete case for expression (25) can be written as

$$W = T^* \oint_c (p_\alpha^{(s)i} \Delta\psi_{(s)i}^\alpha - H_c \Delta t) = \text{inv}. \tag{33}$$

When $\Delta V_i \to 0, \psi_{(s)i}^\alpha(t) \to \psi_{(s)}^\alpha(\boldsymbol{x},t)$, $\pi_\alpha^{(s)i}(t) \to \pi_\alpha^{(s)}(\boldsymbol{x},t)$, the continuous limit of (33) converts into expression (25) (or (32)). Using this result, it is easy to extend the conclusion of the discrete system to the system in the field theories [6].

Let us first consider the quantal equations of motion of the discrete regular Lagrangian in the phase space which is given by [3]. (Similar to the analysis of (22)–(24), the operators can be converted to classical numbers.) We have

$$\begin{aligned} \dot\psi_{(s)i}^\alpha &= \frac{\mathrm{d}\psi_{(s)i}^\alpha}{\mathrm{d}t} = Q_{(s)i}^\alpha(t, \psi_{(s)i}^\alpha, p_\alpha^{(s)i}), \\ \dot p_\alpha^{(s)i} &= \frac{\mathrm{d}p_\alpha^{(s)i}}{\mathrm{d}t} = P_\alpha^{(s)i}(t, \psi_{(s)i}^\alpha, p_\alpha^{(s)i}). \end{aligned} \tag{34}$$

From (25), we can obtain

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t} W' \\ &= \oint_c \left(\frac{\mathrm{d}p_\alpha^{(s)i}}{\mathrm{d}t} \Delta\psi_{(s)i}^\alpha + p_\alpha^{(s)i} \frac{\mathrm{d}}{\mathrm{d}t} \Delta\psi_{(s)i}^\alpha - \frac{\mathrm{d}H_c}{\mathrm{d}t}\Delta t - H_c \frac{\mathrm{d}}{\mathrm{d}t}\Delta t \right) \\ &= \oint_c \left[\frac{\mathrm{d}p_\alpha^{(s)i}}{\mathrm{d}t} \left(\delta\psi_\alpha^{(s)i} + \dot\psi_{(s)i}^\alpha \Delta x^0 \right) \right. \\ &\qquad \left. + p_\alpha^{(s)i} \frac{\mathrm{d}}{\mathrm{d}t} (\delta\psi_\alpha^{(s)i} + \dot\psi_{(s)i}^\alpha \Delta x^0) - \frac{\mathrm{d}H_c}{\mathrm{d}t}\Delta t \right]. \end{aligned} \tag{35}$$

Integrating by parts the terms in (35), one obtains

$$\begin{aligned} 0 &= \oint_c \left[\frac{\mathrm{d}p_\alpha^{(s)i}}{\mathrm{d}t} \delta\psi_{(s)i}^\alpha + p_\alpha^{(s)i} \delta \frac{\mathrm{d}}{\mathrm{d}t} \psi_{(s)i}^\alpha - \frac{\mathrm{d}H_c}{\mathrm{d}t}\Delta t \right] \\ &= \oint_c \left[\frac{\mathrm{d}p_\alpha^{(s)i}}{\mathrm{d}t} \delta\psi_{(s)i}^\alpha - \frac{\mathrm{d}\psi_{(s)i}^\alpha}{\mathrm{d}t} \delta p_\alpha^{(s)i} - \frac{\mathrm{d}H_c}{\mathrm{d}t}\delta t \right] = 0. \end{aligned} \tag{36}$$

From (34), one obtains

$$\oint_c \left[P_\alpha^{(s)i} \delta\psi_{(s)i}^\alpha - Q_{(s)i}^\alpha \delta p_\alpha^{(s)i} - \frac{\mathrm{d}H_c}{\mathrm{d}t}\delta t \right] = 0. \tag{37}$$

Due to the contour of the integrating being arbitrary, and the integrand being the variation of the quantity $-H_c(t, \psi_{(s)i}^\alpha, p_\alpha^{(s)i})$,

$$P_\alpha^{(s)i} \delta\psi_{(s)i}^\alpha - Q_{(s)i}^\alpha \delta p_\alpha^{(s)i} - \frac{\mathrm{d}H_c}{\mathrm{d}t}\delta t = -\delta H_c(t, \psi_{(s)i}^\alpha, p_\alpha^{(s)i}). \tag{38}$$

Thus

$$P_\alpha^{(s)i} = -\frac{\partial H_c}{\partial \psi_{(s)i}^\alpha}, \quad Q_{(s)i}^\alpha = \frac{\partial H_c}{\partial p_\alpha^{(s)i}}. \tag{39}$$

This is to say that the equivalence between the quantal canonical equations and the QPCII is proved for the regular higher-order Lagrangian.

One can still proceed in the same way to obtain the equivalence between the quantal canonical equations and the QPCII for the system with a singular higher-order Lagrangian. But in this case, $(\psi_{(s)i}^\alpha, C_a^i, \bar C_a^i, \eta_i^m)$ and $(p_\alpha^{(s)i}, p_i^a, \bar p_i^a)$ should be used instead of $\psi_{(s)i}^\alpha$ and $p_\alpha^{(s)i}$, and H_{eff} should be used instead of H_c.

From the above discussion we can show that a necessary and sufficient condition for the equations of motion to be quantal canonical equations is that the PC integral be invariant at the quantum level.

When $\Delta V_i \to 0$, the continuous limit of (39) converts into (24); thus the equivalence between the QPCII and the quantal canonical equations of the discrete system can be extended to a system with a higher-order Lagrangian in the field theories.

4 The quantal PCII and the canonical transformation

The canonical transformation in field theories can be stated as follows. Suppose the equations of motion of a dynamical system are given by (24). Then the canonical transformation at the quantum level is to be defined as such a transformation of the canonical variables $\psi_{(s)}^\alpha, \pi_\alpha^{(s)}$. We have

$$\begin{aligned} \psi_{(s)}^{\alpha *} &= Q'^\alpha_{(s)}(t, \psi_{(s)}^\alpha, \pi_\alpha^{(s)}), \\ \pi_\alpha^{(s)*} &= P'^{(s)}_\alpha(t, \psi_{(s)}^\alpha, \pi_\alpha^{(s)}), \end{aligned} \tag{40}$$

which leaves the form of (24) of the system invariant. Under the transformation (40), if two quantities $H_c^* = \int_V \mathrm{d}^3x \mathcal{H}_c^*$ (for the system with a singular Lagrangian, H_{eff} should be used instead of H_c) and G exist so that

$$\begin{aligned} &\int_V \mathrm{d}^3x (\pi_\alpha^{(s)} \Delta\psi_{(s)}^\alpha - \mathcal{H}_c \Delta t) \\ &= \int_V \mathrm{d}^3x (\pi_\alpha^{(s)*} \Delta\psi_{(s)}^{\alpha *} - \mathcal{H}_c^* \Delta t) + \Delta G. \end{aligned} \tag{41}$$

Then the transformation is canonical at the quantum level. In fact, one can choose a closed curve in the extended phase space, and from (41) one can obtain

$$\begin{aligned} \oint_c \left[\int_V \mathrm{d}^3x \left(\pi_\alpha^{(s)} \Delta\psi_{(s)}^\alpha - \mathcal{H}_c \Delta t \right) \right. \\ \left. - \int_V \mathrm{d}^3x (\pi_\alpha^{(s)*} \Delta\psi_{(s)}^{\alpha *} - \mathcal{H}_c^* \Delta t) \right] = 0. \end{aligned} \tag{42}$$

If C^* is the closed curve obtained from C by means of the transformation (40), then (42) can be written as

$$\begin{aligned} &\oint_c \int_V \mathrm{d}^3x (\pi_\alpha^{(s)} \Delta\psi_{(s)}^\alpha - \mathcal{H}_c \Delta t) \\ &= \oint_{c''} \int_V \mathrm{d}^3x (\pi_\alpha^{(s)*} \Delta\psi_{(s)}^{\alpha *} - \mathcal{H}_c^* \Delta t)]. \end{aligned} \tag{43}$$

Because the $\psi^{\alpha}_{(s)}$ and $\pi^{(s)}_{\alpha}$ satisfy the equations of motion (24), the left-hand side of (43) is QPCII at the quantum level, i.e. the left-hand side of (43) is invariant under the displacement and deformation of the closed curve C along the tube of the dynamical trajectories given by the solution of (24). Therefore, the right-hand side of (43) will be invariant under the displacement of the closed curve C^* along the tube obtained by means of the transformation (40). That is to say, the right-hand side of (43) is also a QPCII at the quantum level with respect to the transformed new variables. Thus, the transformed trajectories must satisfy the quantal canonical equations for the system with a higher-order Lagrangian in field theories, and therefore, the transformation (40) is canonical at the quantum level [6].

5 Hamilton–Jacobi equations

Now we discuss the connection between the QPCII and the Hamilton–Jacobi equation at the quantum level. From the analysis in Sect. 3, the discrete case for expression (43) can be written as

$$\oint_c (p^{i(s)}_{\alpha}\Delta\psi^{\alpha}_{i(s)} - H_{\rm c}\Delta t) = \oint_{c^*} (p^{i(s)*}_{\alpha}\Delta\psi^{\alpha*}_{i(s)} - H^*_{\rm c}\Delta t). \quad (44)$$

A smoothed function of θ can be expressed as

$$\Lambda(\theta) = \frac{{\rm d}S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{{\rm d}t}\Delta t(\theta) = \frac{{\rm d}\Omega(\theta)}{{\rm d}\theta}. \quad (45)$$

The integral of $\Lambda(\theta)$ along the closed curve C^* must be equal to zero, so (45) can be added to the right of (44):

$$\oint_c (p^{i(s)}_{\alpha}\Delta\psi^{\alpha}_{i(s)} - H_{\rm c}\Delta t) \quad (46)$$
$$= \oint_{c^*} (p^{i(s)*}_{\alpha}\Delta\psi^{\alpha*}_{i(s)} - H^*_{\rm c}\Delta t) + \oint_{c^*}\left(\frac{{\rm d}S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{{\rm d}t}\right)\Delta t.$$

Due to C and C^* being arbitrary closed curves encircling the tube of quantal dynamical trajectories in extended phase space, we have

$$p^{i(s)}_{\alpha}\Delta\psi^{\alpha}_{i(s)} - p^{i(s)*}_{\alpha}\Delta\psi^{*}_{i(s)} - \left(H_{\rm c} - H^*_{\rm c} + \frac{{\rm d}S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{{\rm d}t}\right)\Delta t = 0. \quad (47)$$

Thus, from (43) (similar to the analysis of (22)–(24), the operators can be converted to classical numbers) we have

$$\left(p^{i(s)}_{\alpha} - \frac{\partial S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{\partial\psi^{\alpha}_{i(s)}}\right)\Delta\psi^{\alpha}_{i(s)} - \left(p^{i(s)*}_{\alpha} + \frac{\partial S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{\partial\psi^{\alpha*}_{i(s)}}\right)\Delta\psi^{\alpha*}_{i(s)} + \left[H^*_{\rm c} - \left(H_{\rm c} + \frac{\partial S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{\partial t}\right)\right]\Delta t = 0. \quad (48)$$

Since $\Delta\psi^{\alpha}_{i(s)}$ and $\Delta\psi^{\alpha*}_{i(s)}$ are independent, one obtains

$$p^{i(s)}_{\alpha} = \frac{\partial S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{\partial\psi^{\alpha}_{i(s)}},$$
$$-p^{i(s)*}_{\alpha} = \frac{\partial S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{\partial\psi^{\alpha*}_{i(s)}}, \quad (49)$$

$$H^*_{\rm c} = H_{\rm c} + \frac{\partial S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{\partial t}. \quad (50)$$

Selecting an S and making $H^*_{\rm c} = 0$, the relation (50) gives

$$H_{\rm c}\left[\psi^{\alpha}_{i(s)}, \frac{\partial S}{\partial\psi^{\alpha}_{i(s)}}, t\right] + \frac{\partial S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{\partial t} = 0. \quad (51)$$

This is the Hamilton–Jacobi equation at the quantum level. In this case, the equations of motion become simple because of $H^*_{\rm c} = 0$, since

$$\dot\psi^{\alpha*}_{i(s)} = \frac{\partial H^*_{\rm c}}{\partial p^{i(s)}_{\alpha}} = 0. \quad (52)$$

Thus

$$\psi^{\alpha*}_{i(s)} = \text{const.} \quad (53)$$

The S can easily be interpreted after taking the total time derivative:

$$\frac{{\rm d}S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{{\rm d}t} = \frac{\partial S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{\partial\psi^{\alpha}_{i(s)}}\dot\psi^{\alpha}_{i(s)} + \frac{\partial S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t)}{\partial t} = p^{i(s)}_{\alpha}\dot\psi^{\alpha}_{i(s)} - H_{\rm c}, \quad (54)$$

then

$$S(\psi^{\alpha}_{i(s)},\psi^{\alpha*}_{i(s)},t) = \int L^p{\rm d}t + \gamma; \quad (55)$$

γ is an arbitrary constant. For the system with the singular higher-order Lagrangian, $H_{\rm eff}$ can be used instead of $H_{\rm c}$ and then $L^p_{\rm eff}$ can be used instead of L^p.

When $\Delta V_i \to 0$, the above analysis can be extended to the system with a higher-order Lagrangian in the field theories.

6 Discussion and conclusions

Considering the transformation property of phase-space generating function of the Green function, along the quantal motion trajectories, the QPCII for a system with a regular/singular higher-order Lagrangian in field theories is derived. It is proved that the QPCII is equivalent to the quantal canonical equations; thus the CPCII is generalized to field theories at the quantum level. For the singular Lagrangian system, the QPCII should be determined by the effective Hamiltonian $H_{\rm eff}$ (not the canonical Hamiltonian $H_{\rm c}$), and the $H_{\rm eff}$ involves all constraints and gauge conditions. This is different from all classical theories. In classical theories, the expressions of PCII for a regular system and a singular system are completely similar. The differences are that the variations of the canonical variables for a system with a regular Lagrangian are arbitrary; but for the system with a singular Lagrangian, those variations are restricted by the constraint conditions (the constraint conditions should be invariant under a substantial variation). The expressions of QPCII for the system with a regular Lagrangian and singular Lagrangian are similar when $\Delta t = 0$ at the quantum level.

The conserved quantities corresponding to the classical symmetries perhaps do not exist at the quantum level. For example, in the Noether theorem at the quantum level, due to the existence of the constraints for a system with a singular Lagrangian in the phase space, the effective Hamiltonian H_{eff} is different from the canonical one H_{c}, and the Jacobian of the transformation may not be equal to unity; thus, the relations between classical symmetries and conservation laws not always are preserved in quantum theories [7]. However, the quantal conserved quantities can be obtained if the effective canonical action is invariant under the global transformation in phase space and the Jacobian of the corresponding local transformation is equal to unity [7]. In general, there is a quantum anomaly when the Jacobian of the transformation is not equal to unity. But this case does not occur for the QPCII. Even if the Jacobian of the transformation is not equal to unity, the QPCII can also be derived. This case is different from the quantal first Noether theorem [7]. The cause arises from the equivalence between the QPCII and the quantal canonical equations. The Hamilton–Jacobi equation can be derived from QPCII at the quantum level.

Recently, the geometric description of symmetries in classical field theory has been formulated [15]. The extension of some results in the above work [15] to quantum theory from the point of view of the ideas developed in this paper needs further discussion.

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